

Niclosamide
50-65-7 | DTXSID7040362

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.87 | 0.81 | 0.87 | 0.82 | 0.86 | 0.86 |

Model Results

Predicted value: 8.62e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.50e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

| | | |
|---|--|--|
| <div>Image not found</div> <div>Hexobarbital</div> <div>Measured: 1.84e-03</div> <div>Predicted: 3.61e-03</div> | <div>Image not found</div> <div>Chloramphenicol</div> <div>Measured: 7.74e-03</div> <div>Predicted: 1.53e-02</div> | <div>Image not found</div> <div>Chlorendic acid</div> <div>Measured: 9.00e-03</div> <div>Predicted: 1.07e-02</div> |
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